The weighted vertex PI index

Aleksandar Ilić
Faculty of Sciences and Mathematics, University of Niš, Serbia
e-mail: aleksandari@gmail.com

Nikola Milosavljević
Faculty of Sciences and Mathematics, University of Niš, Serbia
e-mail: nikola5000@gmail.com

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Abstract

The vertex PI index is a distance–based molecular structure descriptor, that recently found numerous chemical applications. In order to increase diversity of this topological index for bipartite graphs, we introduce weighted version defined as $PI_w(G) = \sum_{e=uv \in E}(deg(u) + deg(v))(n_u(e) + n_v(e))$, where $deg(u)$ denotes the vertex degree of u and $n_u(e)$ denotes the number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v. We establish basic properties of $PI_w(G)$, and prove various lower and upper bounds. In particular, the path P_n has minimal, while the complete tripartite graph $K_{n/3,n/3,n/3}$ has maximal weighed vertex PI index among graphs with n vertices. We also compute exact expressions for the weighted vertex PI index of the Cartesian product of graphs. Finally we present modifications of two inequalities and open new perspectives for the future research.

Key words: PI index; Szeged index; Distance in graphs; Number of triangles; Cartesian product.

AMS Classifications: 05C12, 92E10.

1 Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between u and v in G. The maximum distance in the graph G is its diameter, denoted by d.

In theoretical chemistry molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [8]. There exist several types of such indices, especially those based on vertex and edge distances [18]. Arguably the best known of these indices is the Wiener index W, defined as the sum of distances between all pairs of vertices of the molecular graph [6],

$$W(G) = \sum_{u,v \in V} d(u, v).$$

Besides of use in chemistry, it was independently studied due to its relevance in social science, architecture and graph theory. With considerable success in chemical graph theory, various extensions and generalizations of the Wiener index are recently put forward.

One of the oldest degree-based graph invariants are the first and the second Zagreb indices [9], defined as follows

$$\begin{aligned} M_1(G) &= \sum_{u \in V(G)} deg(v)^2 \\ M_2(G) &= \sum_{uv \in E(G)} deg(u)deg(v). \end{aligned}$$

The Zagreb indices and their variants have been used to study molecular complexity, chirality, in QSPR and QSAR analysis, etc.

Let $e = uv$ be an edge of the graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. The vertex PI index and Szeged index are defined as follows:

$$\begin{aligned} PI(G) &= \sum_{e \in E} n_u(e) + n_v(e) \qquad [3,\ 10,\ 13,\ 24] \\ SZ(G) &= \sum_{e \in E} n_u(e) \cdot n_v(e) \qquad [1,\ 4,\ 11,\ 14,\ 15] \end{aligned}$$

In order to increase diversity for bipartite graphs, we introduce weighted versions of PI and SZ index. In this paper we establish some basic properties of the weighted vertex PI index and prove various lower and upper bounds. We also present modifications of IMO 1984 and IMO 1999 inequalities and use them for establishing a sharp upper bound of weighted PI index. In addition, we compute exact expressions for the weighted vertex PI index of the Cartesian product of graphs and open new perspectives for the future research.

2 Weighted version of vertex PI index

Let P_n and S_n denote the path and the star on n vertices, and let $K_{n,m}$ denote the complete bipartite graph.

We define the weighted version of the vertex PI index as follows

$$PI_w(G) = \sum_{e \in E} (deg(u) + deg(v))(n_u(e) + n_v(e))$$

For bipartite graphs it holds $n_u(e) + n_v(e) = n$, and therefore the diversity of the original PI and SZ indices is not satisfying. The following inequality holds for a graph G with n vertices and m edges [18]

$$PI(G) \leq n \cdot m,$$

with equality if and only if G is bipartite. This is why we introduced weighted version of these indices. Assume that every edge $e = uv$ has weight $deg(v) + deg(u)$. Now, if G is a bipartite graph, we have

$$PI_w(G) = n \sum_{v \in V} deg^2(v). \tag{1}$$

This means that the weighted vertex PI index is directly connected to the first Zagreb index. Furthermore, it follows that among bipartite graphs path P_n and complete bipartite graph

$K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$ have the minimum and maximum value of weighted vertex PI index, respectively [9]. These values are

$$\begin{aligned} PI_w(P_n) &= n(4n-6) \\ PI_w(K_{\lfloor n/2\rfloor,\lceil n/2\rceil}) &= n^2\lfloor n/2\rfloor\lceil n/2\rceil. \end{aligned}$$

Next we present a new formula for computing the weighted vertex PI index of a graph.

Lemma 2.1 *Let G be a connected graph. Then $PI_w(G) = \sum_{x\in V} w_x(G)$, where*

$$w_x = \sum_{e=uv\in E,\ d(x,v)\neq d(x,u)} deg(u) + deg(v).$$

Proof. We apply double counting to the set of ordered pairs (x, e) for which $x \in V(G)$, $e = uv \in E(G)$ and $d(x, v) \neq d(x, u)$. Let $n_e(G) = |\{x \in G \mid d(x, v) \neq d(x, u)\}|$. Then by definition it follows $PI_w(G) = \sum_{e\in E} n_e(G) \cdot (deg(u) + deg(v))$. On the other hand, we have $\sum_{e\in E} n_e(G) \cdot (deg(u) + deg(v)) = \sum_{x\in V} w_x(G)$ and $PI_w(G) = \sum_{x\in V} w_x(G)$, as desired. ■

3 Lower bounds

Theorem 3.1 *Let G be a connected graph on n vertices, m edges and diameter d. Then,*

$$PI_w(G) \geq 4d^2 - 4d - 2 + 6m,$$

with equality if and only if $G \cong P_n$.

Proof. For $n = 2$, inequality is obvious. Otherwise, for each edge $e = uv \in E(G)$, we have $n_u(e) + n_v(e) \geq 2$ and $deg(u) + deg(v) \geq 3$. Let $P_{d+1} = v_0v_1 \ldots v_d$ be a diametrical path. Since the distance of the vertices v_i and v_j in the graphs G and induced subgraph P_{d+1} is equal to $|i - j|$, we have

$$\begin{aligned} PI_w(G) &= \sum_{e\in E(P_{d+1})\cup E(G)\setminus E(P_{d+1})} (deg(u) + deg(v))(n_u(e) + n_v(e)) \\ &\geq PI_w(P_{d+1}) + \sum_{e\in E(G)\setminus E(P_{d+1})} (deg(u) + deg(v))(n_u(e) + n_v(e)) \\ &\geq (d + 1)(4d - 2) + 2 \cdot 3 \cdot (m - d) \\ &= 4d^2 - 4d - 2 + 6m. \end{aligned}$$

The equality holds if and only if there are no other vertices than those from P_{d+1} and since G is connected – it follows that $G \cong P_n$. ■

Theorem 3.2 *Let G be a connected graph on n vertices. Then,*

$$PI_w(G) \geq n(4n - 6),$$

with equality if and only if $G \cong P_n$.

Proof. Let v be an arbitrary vertex from G. Denote with $d = \max\{d(v,u) | u \in G\}$ the eccentricity of v, and define layers

$$L_i(v) = \{u \in V(G) \mid d(v,u) = i\}, \qquad i = 0, 1, \ldots, d.$$

This layer representation of a graph is the main idea of the breadth first search algorithm for graph traversals [2]. The graph G has exactly two types of edges: the edges between vertices of L_i, $0 \leqslant i \leqslant d$, and the edges connecting the vertices of L_i and those of L_{i+1}, $0 \leqslant i \leqslant d-1$. Let H denote the subgraph induced by the edges of the second type. From Lemma 2.1, it follows that each vertex v contributes to $PI_w(G)$ exactly for the sum of weights of the edges of the second type (we can ignore the edges connecting the vertices from the same layer). Notice that $deg_H(u) \leq deg(u)$ and that H is bipartite. Therefore

$$\begin{aligned} w_v &= \sum_{uv \in E(H)} (deg(u) + deg(v)) \\ &\geq \sum_{uv \in E(H)} (deg_H(u) + deg_H(v)) \\ &= \sum_{v \in V} deg_H^2(v) \geq 4n - 6, \end{aligned}$$

since $4n-6$ is the minimum value of the first Zagreb index. Equality holds if and only if G has no edges of the first type and H is isomorphic to P_n. Finally, we have $PI_w(G) = \sum_{v \in V} w_v \geq n(4n-6)$ with equality if and only if $G \cong P_n$. ■

4 Upper bounds

Let $e = uv$ be an arbitrary edge, such that it belongs to exactly $t(e)$ triangles. In that case, it easily follows

$$n_u(e) + n_v(e) \leq n - t(e) \qquad \text{and} \qquad deg(u) + deg(v) \leq n + t(e).$$

Therefore,

$$PI_w(G) \leq \sum_{e \in E} (n - t(e))(n + t(e)) = n^2 m - \sum_{e \in E} t^2(e). \tag{2}$$

A complete multipartite graph $K_{n_1, n_2, \ldots, n_k}$ is a graph in which vertices are adjacent if and only if they belong to different partite sets. Let $T_{n,r}$ be the Turán graph which is a complete r–partite graph on n vertices whose partite sets differ in size by at most one. This famous graph appears in many extremal graph theory problems [28]. Nikiforov in [25] established a lower bound on the minimum number of r-cliques in graphs with n vertices and m edges (for $r = 3$ and $r = 4$). Fisher in [7] determined sharp lower bound for the number of triangles, while Razborov in [27] determined asymptotically the minimal density of triangles in a graph of given edge density.

Theorem 4.1 *Let G be a connected graph on n vertices, m edges and t triangles. Then,*

$$PI_w(G) \leq n^2 m - \frac{9t^2}{m}, \tag{3}$$

with equality if and only if $G \cong K_{a,b}$ for $t = 0$, and $G \cong T_{n,r}$ for $r \mid n$ and $t > 0$.

Proof. The inequality directly follows from (2), by applying Cauchy–Schwarz inequality

$$\sum_{e\in E} 1^2 \sum_{e\in E} t^2(e) \geq \left(\sum_{e\in E} t(e)\right)^2 = (3t)^2,$$

since every triangle is counted exactly 3 times. The equality holds if and only if $t(e) = t'$ for every edge $e = uv \in E$.

Therefore, using (2) it follows that the equality in (3) holds if and only if $n_u(e)+n_v(e) = n-t'$ and $deg(u) + deg(v) = n + t'$ holds for all edges $e \in E$.

For $t = 0$, we have $PI_w(G) = n^2m$ if and only if G is a complete bipartite graph $K_{a,b}$, $a + b = n$. In order to prove this, let $e = uv$ be an arbitrary edge of G. Since $t = 0$ implies $deg(u) + deg(v) = n$ and there are no triangles, the neighbors of u form one independent vertex partition and the neighbors of v form the other independent vertex partition of a bipartite graph $K_{a,b}$. Again, using $deg(x)+deg(y) = n$ for an arbitrary edge xy, it follows that each vertex of G is adjacent to all vertices from other partition and therefore $K_{a,b}$ is a complete bipartite graph.

Assume now that $t > 0$. Let v be a vertex from $V(G)$ with neighbors $N(v) = \{v_1, v_2, \ldots, v_s\}$. Each vertex v_i is adjacent to all vertices that are not adjacent with v. Let $U = V(G) \setminus N(v)$ and assume that there is an edge e incident with the vertices from U. In that case, the number of triangles for that edge $t(e)$ is greater than or equal to s, which is impossible since $t(e) = t(vv_1) \leq s - 1$. Therefore, the vertices from U form an independent set. Let $u \neq v$ be an arbitrary vertex from U. Since G is connected, u is adjacent with some vertex $v_i \in N(v)$ and since $deg(u) + deg(v_i) = n + t' = deg(v) + deg(v_i)$, it follows that $deg(u) = deg(v)$ and $N(u) = N(v)$. Finally, every vertex from U is adjacent with every vertex in $N(v)$.

The vertex v was arbitrary chosen, and it follows that G is isomorphic to a complete multipartite graph $K_{n_1,n_2,\ldots,n_r}$. Since each edge belongs to exactly t' triangles, it easily follows that $n_1 = n_2 = \ldots = n_r = k$. For $r \mid n$, we have

$$|E(T_{n,r})| = \left(1 - \frac{1}{r}\right)\frac{n^2}{2} \qquad \text{and} \qquad t(T_{n,r}) = \frac{n(n-n/r)(n-2n/r)}{6}$$

and

$$PI_w(T_{n,r}) = \left(1 - \frac{1}{r}\right)\frac{n^2}{2} \cdot 2\left(n - \frac{n}{r}\right) \cdot 2\frac{n}{r} = n^2m - \frac{9t^2}{m}.$$

This completes the proof. ■

Next we will establish a sharp upper bound for the weighed PI index. For that we need some preliminary results.

The following lemma is strongly connected to Problem 1 of International Olympiad in Mathematics 1984 [5].

Lemma 4.2 *Let a, b, c be positive real numbers, such that $a + b + c = 1$. Then,*

$$0 \leq ab + bc + ac - abc \leq \frac{8}{27}.$$

Proof. From Cauchy–Schwarz inequality it follows

$$(a + b + c)\left(\frac{1}{a} + \frac{1}{b} + \frac{1}{c}\right) \geq 9,$$

and $ab+bc+ac \geq 9abc \geq abc$. For the right-side inequality, using AM–GM inequality we have

$$\begin{aligned} f(a,b,c) &= ab+bc+ac-abc = c(a+b)+ab(1-c) \leq c(1-c)+\frac{(a+b)^2}{4}(1-c) \\ &= (1-c)\cdot\frac{1+c}{2}\cdot\frac{1+c}{2} \leq \left(\frac{1-c+\frac{1+c}{2}+\frac{1+c}{2}}{3}\right)^3 = \left(\frac{2}{3}\right)^3 = \frac{8}{27}. \end{aligned}$$

with equality if and only if $a=b$ and $1-c=\frac{1+c}{2}$, i.e. $a=b=c=\frac{1}{3}$. ■

Lemma 4.3 *Let $a_1 \geq a_2 \geq \ldots \geq a_n \geq X > 0$ be positive real numbers, such that $a_1+a_2+\ldots+a_n = Y$ and $n \geq 2$. Then*

$$\sum_{i=1}^{n} {a_i}^2 \leq (Y-X)^2 + X^2,$$

with equality if and only if $n=2$ and $a_1 = Y-X$, $a_2 = X$.

Proof. Notice first that $Y-(n-1)X \geq X$. Suppose that $S(a) = \sum_{i=1}^{n} {a_i}^2$ reaches its maximum for some n-tuple $(a_1,a_2,\ldots,a_n) \neq (Y-(n-1)X, X, \ldots, X)$. Then, there exist indices $i \neq j$ such that $a_j \geq a_i > X$. Let $\Delta = a_i - X$. By taking $a'_j = a_j + \Delta$ and $a'_i = a_i - \Delta$, we increase the value of $S(a)$ since ${a'_i}^2 + {a'_j}^2 - ({a_i}^2 + {a_j}^2) = 2\Delta^2 + 2\Delta(a_j - a_i) > 0$. This is clearly a contradiction.

Therefore for fixed n, the maximum is achieved for $a_1 = Y-(n-1)X$ and $a_i = X$, $i = 2,3,\ldots,n$, and its value is $S = (Y-(n-1)X)^2 + (n-1)X^2$. For $1 \leq k \leq n-1$ let $S_k = (Y-kX)^2 + kX^2$. Since $S_{k-1} - S_k = 2(Y-kX)X > 0$, we get

$$S = S_{n-1} < S_{n-2} < \ldots < S_1 = (Y-X)^2 + X^2,$$

which completes the proof. ■

The following theorem is strongly connected to Problem 2 of International Olympiad in Mathematics 1999 [5].

Theorem 4.4 *Let $a_1 \geq a_2 \geq \ldots \geq a_n$ be positive real numbers, such that $a_1+a_2+\ldots+a_n = 1$. Then,*

$$\sum_{i<j} a_i a_j (a_i + a_j)(2 - a_i - a_j) \leq \frac{8}{27},$$

with equality if and only if $a_1 = a_2 = a_3 = \frac{1}{3}$ and $a_4 = \ldots = a_n = 0$.

Proof. Let

$$F(a_1,a_2,\ldots,a_n) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} a_i a_j (a_i + a_j)(2 - a_i - a_j).$$

First, we show the following inequality

$$F(a_1,a_2,\ldots,a_n) \leq F(a_1,a_2,\ldots,a_{n-1}+a_n,0) \tag{4}$$

for all $n \geq 4$. If $a_{n-1} = 0$ or $a_n = 0$, the inequality is obvious. Otherwise, we have

$$\begin{aligned}
\Delta &= F(a_1, a_2, \ldots, a_n) - F(a_1, a_2, \ldots, a_{n-1} + a_n, 0) \\
&= \sum_{i=1}^{n-2} a_i a_n (a_i + a_n)(2 - a_i - a_n) + \sum_{i=1}^{n-2} a_i a_{n-1}(a_i + a_{n-1})(2 - a_i - a_{n-1}) \\
&\quad + a_{n-1} a_n (a_{n-1} + a_n)(2 - a_{n-1} - a_n) \\
&\quad - \sum_{i=1}^{n-2} a_i (a_{n-1} + a_n)(a_i + a_{n-1} + a_n)(2 - a_i - a_{n-1} - a_n) \\
&= \sum_{i=1}^{n-2} a_i a_{n-1} a_n (-4 + 4a_i + 3a_{n-1} + 3a_n) + a_{n-1} a_n (a_{n-1} + a_n)(2 - a_{n-1} - a_n) \\
&= a_{n-1} a_n \left[-4 \sum_{i=1}^{n-2} a_i + 4 \sum_{i=1}^{n-2} {a_i}^2 + 3(a_{n-1} + a_n) \sum_{i=1}^{n-2} a_i + 2(a_{n-1} + a_n) - (a_{n-1} + a_n)^2 \right]
\end{aligned}$$

Let $x = a_{n-1}$ and $y = a_n$. Using $\sum_{i=1}^{n-2} a_i = 1 - a_{n-1} - a_n = 1 - x - y$, we get

$$\Delta = xy(-4 + 4 \sum_{i=1}^{n-2} {a_i}^2 + 9x + 9y - 4(x + y)^2).$$

Therefore, $\Delta \leq 0$ is equivalent to

$$\sum_{i=1}^{n-2} {a_i}^2 \leq 1 + (x + y)^2 - \frac{9}{4}(x + y).$$

Next, we will consider the following two cases.

Case 1. $n = 4$.

Using $x + y = 1 - a_1 - a_2$ we get

$$\sum_{i=1}^{n-2} {a_i}^2 \leq 1 + (x + y)^2 - \frac{9}{4}(x + y) \quad \Leftrightarrow \quad a_1 + a_2 + 8a_1 a_2 \geq 1.$$

By ordering we have $a_2 \geq \frac{1 - a_1}{3}$ and after substitution it suffices to prove $(a_1 - 1)(4a_1 - 1) \leq 0$ which is true because $1 \geq a_1 \geq \frac{1}{4}$.

Equality occurs only for $(a_1, a_2, a_3, a_4) = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, since we exclude the case $(1, 0, 0, 0)$ because of the assumption $y \neq 0$.

Case 2. $n > 4$.

By applying Lemma 4.3 on $a_1, \ldots, a_{n-2}$ with $X = x$ and $Y = 1 - x - y$, we get

$$\sum_{i=1}^{n-2} {a_i}^2 < (1 - 2x - y)^2 + x^2.$$

Now, it suffices to prove

$$(1 - 2x - y)^2 + x^2 \leq 1 + (x + y)^2 - \frac{9}{4}(x + y).$$

Simplification gives $7x \geq 16x^2 + 8xy + y$, which can be easily verified using $x \geq y$ and $x \leq \frac{1}{4}$.

With this, inequality (4) is proven. Notice that inequality is strict unless $a_n = 0$, or $n = 4$ and $(a_1, a_2, a_3, a_4) = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. Using this inequality and induction, we can reduce the problem to $n = 3$,

$$F(a_1, a_2, a_3) = \sum_{1 \leq i < j \leq 3} a_i a_j (1 - a_{6-i-j})(1 + a_{6-i-j}) = a_1 a_2 + a_2 a_3 + a_3 a_1 - a_1 a_2 a_3.$$

Now the result follows directly from Lemma 4.2 and $F(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}) = \frac{9}{32} < \frac{8}{27}$. ■

The value of weighted PI index of complete multipartite graph can be easily calculated,

$$PI_w(K_{n_1, n_2, \ldots, n_k}) = \sum_{i<j} n_i n_j (n_i + n_j)(2n - n_i - n_j).$$

By substituting $a_i = \frac{n_i}{n}$ and applying Theorem 4.4, it follows that among all multipartite graphs, the balanced 3-partite graph $K_{\lfloor n/3 \rfloor, \lceil n/3 \rceil, n - \lfloor n/3 \rfloor - \lceil n/3 \rceil}$ is the unique graph with maximum weighted vertex PI index. Indeed, maximum is achieved for some partition of size 3. The case $3 \mid n$ follows directly from Theorem 4.4; otherwise assume that (n_1, n_2, n_3) is some 3-partition with $n_3 - n_1 \geq 2$. It can be easily verified that

$$PI_w(K_{n_1, n_2, n_3}) - PI_w(K_{n_1+1, n_2, n_3-1}) = n(n - n_2)(n_1 + 1 - n_3) < 0,$$

which means that (n_1, n_2, n_3) is balanced.

For $3 \mid n$ it holds $PI_w(K_{n/3, n/3, n/3}) = \frac{8}{27} n^4$. We now show that $\frac{8}{27} n^4$ is the upper bound for $PI_w(G)$ among all graphs on n vertices and that this bound is sharp for $3 \mid n$.

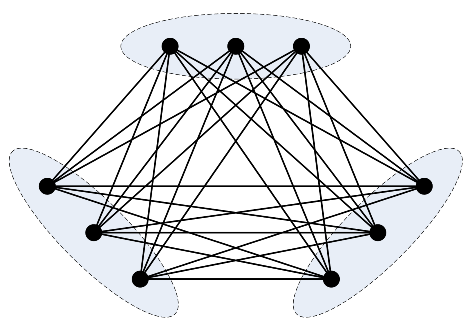

Figure 1: The complete tripartite graph $K_{3,3,3}$.

Theorem 4.5 *Let G be a connected graph on n vertices. Then,*

$$PI_w(G) \leq \frac{8}{27} n^4,$$

with equality if and only if $3 \mid n$ and $G \cong K_{n/3, n/3, n/3}$.

Proof. Let $G_{n,m}$ be connected graph on n vertices and m edges. Denote by $t_{n,m}$ the smallest possible number of triangles in $G_{n,m}$. From Theorem 4.1 it follows that

$$PI_w(G_{n,m}) \leq n^2 m - \frac{9t^2}{m} \leq n^2 m - \frac{9t_{n,m}^2}{m}$$

In [26] the authors proved that

$$t_{n,m} \geq \frac{(4m - n^2)m}{3n}$$

with equality if and only if G is a complete multipartite graph with partitions of equal size. Substituting this in the previous inequality and after some simplification, we get

$$PI_w(G_{n,m}) \leq 8 \cdot \frac{n^2m^2 - 2m^3}{n^2}.$$

It suffices to prove that $8 \cdot \frac{n^2m^2-2m^3}{n^2} \leq \frac{8}{27}n^4$, which is equivalent to $n^6 + 54m^3 \geq 27n^2m^2$. This is true by simple AM–GM inequality:

$$\left(\frac{n^2}{3}\right)^3 + m^3 + m^3 \geq n^2m^2,$$

with equality if and only if $m = \frac{n^2}{3}$. It follows that $PI_w(G_{n,m}) \leq \frac{8}{27}n^4$ for all $n-1 \leq m \leq \binom{n}{2}$, and therefore $PI_w(G) \leq \frac{8}{27}n^4$ as desired. From the above analysis, the equality holds if and only if G is a regular multipartite graph with partitions of size $\frac{n}{3}$. ■

5 Cartesian product graphs

In this section we present formulas for computing weighted PI index of the Cartesian product of graphs. In [21, 22, 19] the authors computed the PI index, the vertex PI index and the Szeged index of Cartesian product graphs, respectively.

For graphs G and H, the Cartesian product $G \times H$ is a graph with vertex set $V(G \times H) = V(G) \times V(H)$ and $(u', u'')(v', v'')$ is an edge of $G \times H$ if $u' = v'$ and $u''v'' \in E(H)$, or $u'v' \in V(G)$ and $u'' = v''$. We will use the following well-known assertions for the Cartesian product of graphs (see book of Imrich and Klavžar [16] for more details) and vertices $u = (u', u'')$, $v = (v', v'')$:

- $|V(G \times H)| = |V(G)| \cdot |V(H)|$
- $|E(G \times H)| = |V(G)||E(H)| + |V(H)||E(G)|$
- $deg_{G \times H}(u) = deg_G(u') + deg_H(u'')$
- $d_{G \times H}(u, v) = d_G(u', v') + d_H(u'', v'')$.

Let us recall alternative formulas for computing the vertex and weighted PI index (see Lemma 2.1 and [24]): $PI_v(G) = \sum_{x \in G} m_x(G)$ and $PI_w(G) = \sum_{x \in G} w_x(G)$, where

$$\begin{aligned} w_x(G) &= \sum_{e=uv \in E(G),\ d(x,v) \neq d(x,u)} deg(u) + deg(v), \\ m_x(G) &= \sum_{e=uv \in E(G),\ d(x,v) \neq d(x,u)} 1. \end{aligned}$$

Theorem 5.1 *Let G and H be two connected graphs. Then*

$$PI_w(G \times H) = |V(G)|^2 PI_w(H) + |V(H)|^2 PI_w(G) + 4\Big(|V(G)||E(G)|PI_v(H) + |V(H)||E(H)|PI_v(G)\Big).$$

Proof. We will use the formula

$$PI_w(G \times H) = \sum_{x \in V(G \times H)} w_x(G \times H).$$

Notice that for $x, u, v \in G \times H$, the condition $d(x,u) \neq d(x,v)$ is equivalent with

$$d((x', x''), (u', u'')) \neq d((x', x''), (v', v'')) \Leftrightarrow d(x', u') + d(x'', u'') \neq d(x', v') + d(x'', v'').$$

If $(u, v) \in E(G \times H)$ it follows the either $u' = v'$ or $u'' = v''$, and therefore

$$\begin{aligned} w_x(G \times H) &= \sum_{e=uv \in E(G\times H),\ d(x,v)\neq d(x,u)} deg(u) + deg(v) \\ &= \sum_{u''v'' \in E(H),\ u'=v',\ d(x'',v'')\neq d(x'',u'')} deg(u') + deg(v') + deg(u'') + deg(v'') + \\ &\quad \sum_{u'v' \in E(G),\ u''=v'',\ d(x',v')\neq d(x',u')} deg(u') + deg(v') + deg(u'') + deg(v'') \\ &= A(x) + B(x). \end{aligned}$$

We have

$$\begin{aligned} A(x) &= \sum_{u' \in G} \sum_{u''v'' \in E(H),\ d(x'',v'')\neq d(x'',u'')} 2 \cdot deg(u') + deg(u'') + deg(v'') \\ &= \sum_{u' \in G} (m_{x''}(H) \cdot 2 \cdot deg(u') + w_{x''}(H)) \\ &= 4|E(G)| m_{x''}(H) + |V(G)| w_{x''}(H). \end{aligned}$$

Analogously, $B(x) = 4|E(H)| m_{x'}(G) + |V(H)| w_{x'}(G)$ and thus

$$w_x(G \times H) = |V(G)| w_{x''}(H) + |V(H)| w_{x'}(G) + 4|E(G)| m_{x''}(H) + 4|E(H)| m_{x'}(G).$$

Finally, it follows

$$\begin{aligned} PI_w(G \times H) &= \sum_{x' \in V(G),\ x'' \in V(H)} A(x) + B(x) \\ &= |V(G)| \sum_{x'' \in V(H)} A(x) + |V(H)| \sum_{x' \in V(G)} B(x) \\ &= |V(G)|(4|E(G)| PI_v(H) + |V(G)| PI_w(H)) \\ &\quad + |V(H)|(4|E(H)| PI_v(G) + |V(H)| PI_w(G)), \end{aligned}$$

which completes the proof. ■

Denote by $\bigotimes_{i=1}^n G_i$ the Cartesian product of graphs $G_1 \times G_2 \times \ldots \times G_n$ and let $|V(G_i)| = V_i$ and $|E(G_i)| = E_i$ for all $i = \overline{1,n}$. Using the above properties of Cartesian product graphs, one can easily verify that $V(\bigotimes_{i=1}^n G_i) = \prod_{i=1}^n V_i$ and $E(\bigotimes_{i=1}^n G_i) = \sum_{i=1}^n E_i \prod_{j=1,\ j\neq i}^n V_i$. In [19], Khalifeh et al. have proven

$$PI_v(\bigotimes_{i=1}^n G_i) = \sum_{i=1}^n PI_v(G_i) \prod_{j=1,\ j\neq i}^n |V(G_j)|^2. \tag{5}$$

We prove similar result for weighted PI index:

Theorem 5.2 *Let $G_1, G_2, \ldots, G_n$ be connected graphs. Then*

$$PI_w(\bigotimes_{i=1}^n G_i) = \sum_{i=1}^n PI_w(G_i) \prod_{j=1,\ j\neq i}^n V_j^2 + 4 \sum_{i,j=1,\ i\neq j}^n PI_v(G_i) V_j E_j \prod_{k=1, i\neq k\neq j}^n V_k^2.$$

Proof. The case $n = 2$ was proven in Theorem 5.1. We continue our argument by mathematical induction. Suppose that the result is valid for some n graphs. Using Theorem 5.1 and equation (5) we have

$$
\begin{aligned}
PI_w(\bigotimes_{i=1}^{n+1} G_i) &= PI_w(\bigotimes_{i=1}^{n} G_i \times G_{n+1}) \\
&= |V(\bigotimes_{i=1}^{n} G_i)|^2 PI_w(G_{n+1}) + V_{n+1}^2 PI_w(\bigotimes_{i=1}^{n} G_i) \\
&\quad +4\Big(|V(\bigotimes_{i=1}^{n} G_i)||E(\bigotimes_{i=1}^{n} G_i)|PI_v(G_{n+1}) + V_{n+1}E_{n+1}PI_v(\bigotimes_{i=1}^{n} G_i)\Big) \\
&= PI_w(G_{n+1})\prod_{i=1}^{n} V_i{}^2 + V_{n+1}^2 \sum_{i=1}^{n} PI_w(G_i) \prod_{j=1,\ j\neq i}^{n} V_i^2 \\
&\quad +4 \sum_{i,j=1,\ i\neq j}^{n} PI_v(G_i)V_jE_j \prod_{k=1,i\neq k\neq j}^{n+1} V_k^2 \\
&\quad +4\Big(PI_v(G_{n+1})\sum_{i=1}^{n} E_iV_i \prod_{j=1,\ j\neq i}^{n} V_j^2 + V_{n+1}E_{n+1}\sum_{i=1}^{n} PI_v(G_i) \prod_{j=1,\ j\neq i}^{n} V_j^2\Big) \\
&= \sum_{i=1}^{n+1} PI_w(G_i) \prod_{j=1,\ j\neq i}^{n+1} V_j{}^2 \\
&\quad +4\Big(\sum_{i,j=1,\ i\neq j}^{n} PI_v(G_i)V_jE_j \prod_{k=1,i\neq k\neq j}^{n+1} V_k^2 + \sum_{\substack{1\leq i,j\leq n \\ i=n+1\vee j=n+1}} PI_v(G_i)V_jE_j \prod_{k=1,i\neq k\neq j}^{n+1} V_k^2\Big) \\
&= \sum_{i=1}^{n+1} PI_w(G_i) \prod_{j=1,\ j\neq i}^{n+1} V_j{}^2 + 4 \sum_{i,j=1,\ i\neq j}^{n+1} PI_v(G_i)V_jE_j \prod_{k=1,i\neq k\neq j}^{n+1} V_k{}^2.
\end{aligned}
$$

This completes the proof. ■

Corollary 5.3 *Let G be connected graph. Then*

$$PI_w(G^n) = PI_w(\bigotimes_{i=1}^{n} G) = n|V(G)|^{2n-3}\Big(|V(G)|PI_w(G) + 4(n-1)|E(G)|PI_v(G)\Big).$$

Proof. Directly follows from Theorem 5.2. ■

6 Concluding remarks

The vertex PI and Szeged indices are novel molecular-structure descriptors. In this paper we generalized these indices and open new perspectives for the future research. Similarly we can define weighted Szeged index as follows

$$SZ_w(G) = \sum_{e\in E}(deg(u) + deg(v))n_u(e) \cdot n_v(e).$$

It would be interesting to study mathematical properties of these modified indices and report their chemical relevance and formulas for some important graph classes. In particular, some exact expressions for the weighted PI and SZ index of other graph operations (such as the composition, join, disjunction and symmetric difference of graphs, bridge graphs, Kronecker product of graphs) can be derived, similarly as in [12, 20, 21, 23].

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